March 6, 2016

$$H' = -\frac{1}{8m^2c^2} p^4$$

$$H^0 = \frac{p^2}{2m} + V(r)$$

$$p^2 |nlm\rangle = 2m(E-V)|nlm\rangle$$

$$\langle nlm|p^4|nlm\rangle = \langle nlm|[2m(E-V)]^2|nlm\rangle \Leftarrow$$

$$\Rightarrow p^2 \; 2m(E-V)|nlm\rangle \neq 2m(E-V)p^2|nlm\rangle$$
$$= [2m(E-V)]^2|nlm\rangle$$

$$\langle nlm|p^4|nlm\rangle = |p^2|nlm\rangle|^2$$
$$= (\langle nlm|p^2)(p^2|nlm\rangle)$$

$$p^2 \, 2m(E-V)|nlm\rangle = 2m(E-V)p^2|nlm\rangle$$
$$+[p^2, 2m(E-V)]|nlm\rangle$$

$$\langle nlm|[p^2, 2m(E-V)]|nlm\rangle \stackrel{?}{=} 0$$

$$[p^2, 2m(E-V)] = -2m[p^2, V]$$
$$= -2m\{\vec{p}\cdot\underbrace{[\vec{p}, V]} + [\vec{p}, V]\cdot\vec{p}\}$$

$$[\vec{p}, V]\psi = \vec{p}(V\psi) - V(\vec{p}\psi)$$
$$= -i\hbar\vec{\nabla}(V\psi) - V(-i\hbar\vec{\nabla}\psi)$$
$$= (-i\hbar\vec{\nabla}V)\psi + \cancel{V(-i\hbar\vec{\nabla}\psi)} - \cancel{V(-i\hbar\vec{\nabla}\psi)}$$

$$[\vec{p}, V] = -i\hbar(\vec{\nabla}V)$$

$$[p^2, 2m(E-V)] = -2m\{\vec{p}\cdot(-i\hbar\vec{\nabla}V) + (-i\hbar\vec{\nabla}V)\cdot\vec{p}\}$$

$$= -2m\{2(-i\hbar\vec{\nabla}V)\cdot\vec{p} + -i\hbar[\vec{p}, \vec{\nabla}V]\}$$

$$= -2m\{-2i\hbar(\vec{\nabla}V)\cdot\vec{p} + (-i\hbar)^2\nabla^2 V\}$$

$$V = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$

$$\vec{\nabla}V = -\frac{e^2}{4\pi\varepsilon_0}\frac{\hat{r}}{r^2} \qquad \nabla^2 V = -e^2\frac{\delta^3(\vec{r})}{\varepsilon_0}$$

$$\underline{[p^2, 2m(E-V)]} = -2m\left\{-2i\hbar\left(\frac{-e^2}{4\pi\varepsilon_0}\right)\left(\frac{\hat{r}\cdot\vec{p}}{r^2}\right) + (-i\hbar)^2\frac{(-e^2)}{\varepsilon_0}\delta^3(\vec{r})\right\}$$

$$\langle nlm|\frac{\hat{r}}{r^2}\cdot\vec{p}|nlm\rangle$$

$$= \int d^3r\, \psi^*_{nlm}(\vec{r})\frac{1}{r^2}\frac{\partial}{\partial r}\psi_{nlm}(\vec{r})$$

$$= \int_0^\infty dr\, \cancel{r^2}\, R_{nl}(r)\frac{1}{\cancel{r^2}}\frac{\partial}{\partial r}R_{nl}(r)$$

$$= \frac{1}{2}\left(R_{nl}(r)\right)^2\Big|_{r=0}^{\infty}$$

$$= -\frac{1}{2}\left(R_{nl}(0)\right)^2$$

$$R_{nl}(r) \overset{r\to 0}{\simeq} \underline{r^l} \qquad -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

$$\langle nlm|\frac{\hat{r}}{r^2}\cdot\vec{p}|nlm\rangle = 0 \quad \text{if } l \neq 0$$

$\langle nlm | \delta^3(\vec{r}) | nlm \rangle = |\psi_{nlm}(\vec{0})|^2 = 0$ if $l \neq 0$

if $l = 0$

$$\langle n00 | \frac{\hat{r}}{r^2} \cdot \vec{p} | n00 \rangle = -\frac{1}{2} |R_{n0}(0)|^2 (-i\hbar)$$

$$\langle n00 | \delta^3(\vec{r}) | n00 \rangle = |R_{n0}(0)\, Y_{00}(0)|^2$$
$$= |R_{n0}(0)|^2 \frac{1}{4\pi}$$

$$\int d\Omega\, |Y_{00}|^2 = 1$$

$$|Y_{00}|^2 \underbrace{\int d\Omega}_{4\pi} = 1 \Rightarrow |Y_{00}| = \frac{1}{\sqrt{4\pi}}$$

relativistic correction

$$\frac{E_r^{(1)}}{E_n} = -\left(\frac{E_n}{mc^2}\right) \frac{1}{2} \left[\frac{4n}{l+\frac{1}{2}} - 3\right]$$

$$\frac{E_n}{mc^2} \sim 10^{-5} \qquad (kT)_{\substack{\text{room} \\ \text{temperature}}} \simeq \frac{1}{40}\,\text{eV}$$

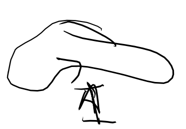
$$E_r^{(1)} \simeq 10^{-5}\, 10\,\text{eV} \sim 10^{-4}\,\text{eV}$$

$$\frac{E_r^{(1)}}{kT} \simeq \frac{10^{-4}\,\text{eV}}{\frac{1}{40}\,\text{eV}} \sim 10^{-2}$$

Spin-Orbit Coupling

Classical Electrodynamics

$$H' = -\underline{\vec{\mu}_e} \cdot \underline{\vec{B}_p}$$



$\mu = IA$

$$\vec{\mu}_e = A \vec{S} \qquad [\mu_e] = \frac{C}{s} m^2$$
$$[\vec{S}] = Js = kg\, m^2/s$$

$$[A] = \left(\frac{C}{\cancel{s}} \cancel{m^2}\right) / \left(kg\, \cancel{m^2} / \cancel{s}\right) = \frac{C}{kg}$$

$$\boxed{\vec{\mu}_e = \frac{q}{m}\vec{S}} \qquad \boxed{\vec{\mu}_e = g_e\frac{q}{2m}\vec{S}} \Leftarrow$$

g_e : gyromagnetic ratio.

$$I = \frac{q}{T}$$

$$\cancel{L} = S = mr\frac{2\pi r}{T}$$

$$\mu = \frac{q(\pi r^2)}{T}$$

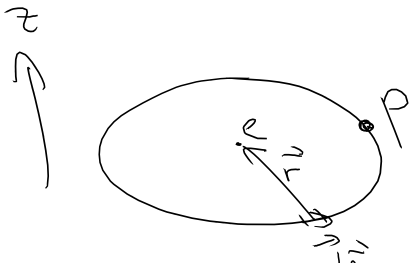
$$\frac{\mu}{S} = \frac{q}{\cancel{T}}(\cancel{\pi r^2})\frac{\cancel{T}}{2\cancel{\pi} m\cancel{r^2}} = \frac{q}{2m}$$

$g_e \approx 2$ (Dirac eqn)

$= 2 + \frac{\alpha}{4\pi}$

Nobel prize por Schwinger

$\vec{B}_p = ?$



$$I = \frac{q_p}{T}$$

$$d\vec{B} = \frac{\mu_0}{4\pi}\frac{I\, d\vec{l}\times\hat{r}}{r^2}$$

$$d\vec{B} = \frac{\mu_0}{4\pi}\frac{q_p}{T}\frac{dl}{r^2}\hat{z}$$

$$\vec{B} = \frac{\mu_0}{2\cancel{4\pi}}\frac{q_p}{T}\frac{\cancel{2\pi} r}{r^{\cancel{2}}}\hat{z}$$

$$\boxed{\vec{B} = \frac{\mu_0}{2r}\frac{q_p}{T}\hat{z}}$$

$$\vec{L}_e = mr^2\frac{2\pi}{T}\hat{z}$$

$$\vec{B} = \frac{\mu_0}{2r}q_p\vec{L}\left(\frac{1}{2\pi m r^2}\right)$$

$$\vec{B} = \frac{\mu_0}{4\pi} \frac{q_p}{m r^3} \vec{L} \qquad c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}$$

$$\boxed{\vec{B} = \frac{1}{4\pi\varepsilon_0} \frac{q_p}{m c^2 r^3} \vec{L}}$$

$$H' = -\left(g_e \frac{q_e}{2m} \vec{S}\right) \cdot \left(\frac{1}{4\pi\varepsilon_0} \frac{q_p}{m c^2 r^3} \vec{L}\right) \left(\frac{1}{2}\right)$$

Thomas precession

For $g_e = 2$

$$\boxed{H' = \underbrace{\frac{+e^2}{4\pi\varepsilon_0}}_{\alpha} \underbrace{\frac{1}{2m^2c^3r^3}} \vec{S} \cdot \vec{L}}$$

$$\left\{ |n l m\rangle \otimes |s m_s\rangle \right\}$$

$$\langle n l s m' m_s' | H' | n l m s m_s \rangle \overset{?}{=} 0 \quad \text{if} \quad \begin{matrix} m \neq m' \\ m_s \neq m_s' \end{matrix} \;?$$

$$L_\pm = \frac{L_x \pm i L_y}{\sqrt{2}} \qquad \vec{S} \cdot \vec{L} = S_+ L_- + \underline{S_- L_+} + S_z L_z$$

$$S_\pm = \frac{S_x \pm i S_y}{\sqrt{2}} \qquad \langle n l s (m+1)(m_s-1) | \vec{S} \cdot \vec{L} | n l m s m_s \rangle \neq 0$$

$$\vec{S} \cdot \vec{L} = \frac{1}{2}\left[(\vec{L} + \vec{S})^2 - L^2 - S^2 \right]$$
$$= \frac{1}{2}\left[\vec{J}^2 - \vec{L}^2 - \vec{S}^2 \right]$$

$$|l s j m_j\rangle$$

$$\vec{J}^2 |l s j m_j\rangle = \hbar^2 j(j+1) |l s j m_j\rangle$$
$$\vec{L}^2 |l s j m_j\rangle = \hbar^2 l(l+1) |l s j m_j\rangle$$
$$\vec{S}^2 |l s j m_j\rangle = \hbar^2 s(s+1) |l s j m_j\rangle$$
$$= \frac{3}{4}\hbar^2 |l s j m_j\rangle$$

$$\{|n\, l\, s\, j\, m_j\rangle\} \Leftarrow$$

$$E^{(1)} = \langle n\, l\, s\, j\, m_j | \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2m^2c^3 r^3} \vec{S}\cdot\vec{L} | n\, l\, s\, j\, m_j\rangle$$

$$E^{(1)} = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2m^2c^3} \left\langle \frac{1}{r^3} \right\rangle_{nl} \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]$$

$$E^{(1)}_{so} = \frac{E_n^2}{mc^2} \left\{ \frac{n\left[j(j+1) - l(l+1) - \frac{3}{4}\right]}{l(l+1)(l+\frac{1}{2})} \right]$$

$$\frac{E^{(1)}_{so}}{E_n} \propto \frac{E_n}{mc^2} \propto E_r^{(1)}$$

$$E^{(1)}_{fs} = \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)$$

Zeeman Effect

$$H'_Z = -\vec{\mu}\cdot\vec{B}_{ext}$$

$$\vec{\mu} = \left(g_e \frac{q}{2m}\vec{S} + \frac{q}{2m}\vec{L}\right)$$

$$\vec{\mu} = -\frac{e}{2m}(\vec{L} + 2\vec{S})$$

$$H'_Z = +\frac{e}{2m}(\vec{L} + 2\vec{S})\cdot\vec{B}_{ext}$$

$$H'_Z = \frac{e}{2m}(\vec{J} + \vec{S})\cdot\vec{B}_{ext}$$

Assume $\vec{B}_{ext} = B_{ext}\hat{z}$

$$H'_Z = \frac{e}{2m} B_{ext} (J_z + S_z)$$

2 limits

$B_{ext} \gg B_{int}$ or $B_{ext} \ll B_{int}$

<u>Weak Zeeman Effect</u> $B_{ext} \ll B_{int}$

$$\{ |n l s j m_j\rangle \} \Leftarrow$$

$$|\psi_n\rangle = |\psi_n\rangle^0 + \sum_{k \neq n} \frac{\langle \psi_k | H' | \psi_n\rangle^0}{E_n^{(0)} - E_k^{(0)}} |\psi_k\rangle^{(0)}$$

$$\langle n l s j m_j | \frac{e}{2m} (\vec{L} + 2\vec{S}) \cdot \vec{B}_{ext} | n l s j m_j \rangle$$

$$= \langle n l s j m_j | \frac{e}{2m} (\vec{J} + \vec{S}) \cdot \vec{B}_{ext} | n l s j m_j \rangle$$

$$\langle J_x \rangle = \langle J_y \rangle = 0$$

$$\langle J_z \rangle = \hbar m_j$$

$$\langle \vec{S} \rangle = ?$$

$$\langle \vec{S}_{av} \rangle = \left\langle \frac{(\vec{S} \cdot \vec{J}) \vec{J}}{J^2} \right\rangle \Leftarrow$$

$$\vec{S} = \underline{(\vec{S} \cdot \hat{J}) \hat{J}} + \text{perpendicular component}$$

$$\vec{S} \cdot \vec{J} = -\frac{1}{2} \Big[\underbrace{(\vec{J} - \vec{S})^2}_{L^2} - \vec{J}^2 - \vec{S}^2 \Big]$$

$$\left\langle \frac{(\vec{S} \cdot \vec{J}) \vec{J}}{J^2} \right\rangle = \frac{\frac{\hbar^2}{2} \left[\frac{4}{3} + j(j+1) - l(l+1) \right]}{\hbar^2 j(j+1)} \langle \vec{J} \rangle$$

$$\vec{B}_{ext} = B_{ext} \hat{z}$$

$$\langle \vec{L} + 2\vec{S} \rangle = \underbrace{\left[1 + \frac{j(j+1) - l(l+1) + \frac{3}{4}}{2j(j+1)} \right]}_{g_J \,:\, \text{Landé } g\text{-factor}} \langle \vec{J} \rangle$$

$$\langle \vec{\mu} \rangle = g_J \frac{q}{2m} \langle \vec{J} \rangle$$

$$\boxed{E_z^{(1)} = g_J \frac{e}{2m} m_j B_{ext}}$$

Strong Zeeman Effect $\quad B_{ext} \gg B_{int}$

$$H' = \frac{e}{2m} B_{ext} (L_z + 2S_z)$$

$$\{ |n l m_l m_s \rangle \}$$

$$\langle n l m_l' m_s' | H' | n l m_l m_s \rangle = \delta_{m_l m_l'} \delta_{m_s m_s'} \frac{\hbar e}{2m} B_{ext} (m_l + 2m_s)$$

$$\langle n l m_l m_s | H_{so} | n l m_l m_s \rangle$$
$$= \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2m^2c^2} \langle n l m_l m_s | \frac{1}{r^3} \vec{S} \cdot \vec{L} | n l m_l m_s \rangle$$
$$= \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2m^2c^2} \left\langle \frac{1}{r^3} \right\rangle \Big\{ \underbrace{\langle S_x \rangle}_{0} \underbrace{\langle L_x \rangle}_{0} + \underbrace{\langle S_y \rangle}_{0} \underbrace{\langle L_y \rangle}_{0} + \langle S_z \rangle \langle L_z \rangle \Big\}$$
$$= \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2m^2c^2} \left\langle \frac{1}{r^3} \right\rangle \hbar^2 m_l m_s$$

Hyperfine Splitting

$$\vec{\mu}_p = g_p \frac{q}{2m_p} \vec{S}_p$$

$$g_p \sim 5$$